Structure of systems of ODE's arising from chemical kinetics

Michael Blinov (April 23, 2003)

There are many systems of ODE's, considered in biology. The simplest and the most often used is the following. Let we are given n species $A_1, A_2, \ldots, A_n$. Then the following are possible reaction classes:

- $A_i \longrightarrow A_j$, rate k_{ij}. There are at most $n(n-1)$ such reactions, as $i \neq j$.
- $A_i + A_j \longrightarrow A_l$, rate k'_{ijl}. There are at most $n(n-1)(n-2)$ such reactions, as i, j should be different from l.
- $A_i \longrightarrow A_j + A_l$, rate k''_{ijl}. There are at most $n(n-1)(n-2)$ such reactions.

We have the system of n equations for species, a typical equation looks like:

$$\begin{aligned}
\frac{dA_s}{dt} &= \sum_{i=1}^{n}(k_{is}A_i - k_{si}A_s) \\
&+ \sum_{i,j=1}^{n} k'_{ijs}A_iA_j - \sum_{i,l=1}^{n}(k'_{isl} + k'_{sil})A_iA_s \\
&+ \sum_{i,j=1}^{n}(k''_{ijs} + k''_{isj})A_i - \sum_{j,l=1}^{n} k''_{sjl}A_s
\end{aligned}$$

Let's notice that to be consistent with the rule that $A_i + A_s$ is symmetric, either $k'_{isl} = 0$ or $k''_{sil} = 0$ and either $k''_{ijs} = 0$ or $k''_{isj} = 0$. This doesn't change the general appearance of the system:

$$\frac{dA_s}{dt} = \sum_{i=1}^{n} K_i^s A_i + \sum_{i,j=1}^{n} K_{ij}^s A_i A_j.$$

In general, rates k's may depend on time and be rather complicated, depending also on participating in a reaction species in a weird manner. But the structure of each equation in general will be the same:

$$\frac{dA_s}{dt} = \sum_{i=1}^{n} F(t, A_i) + \sum_{i,j=1}^{n} G(t, A_i, A_j).$$

Most typical questions:

- Fast solving for large n.
- Limit behavior as time goes to infinity (or zero in some cases).
- Dependence on parameters k (in many aspects: for small perturbations, on a large interval of k, if parameters are related by some relation etc).
- Dependence on initial values $A_s(t_0)$.